



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:11 PM UTC

PDB ID : 8W06 / pdb_00008w06
Title : Crystal Structure of the reconstruction of the ancestral triosephosphate isomerase of the last opisthokont common ancestor obtained by maximum likelihood with PGH
Authors : Perez-Nino, J.A.; Rodriguez-Romero, A.; Guerra-Borrego, Y.; Fernandez-Velasco, D.A.
Deposited on : 2024-02-13
Resolution : 2.06 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

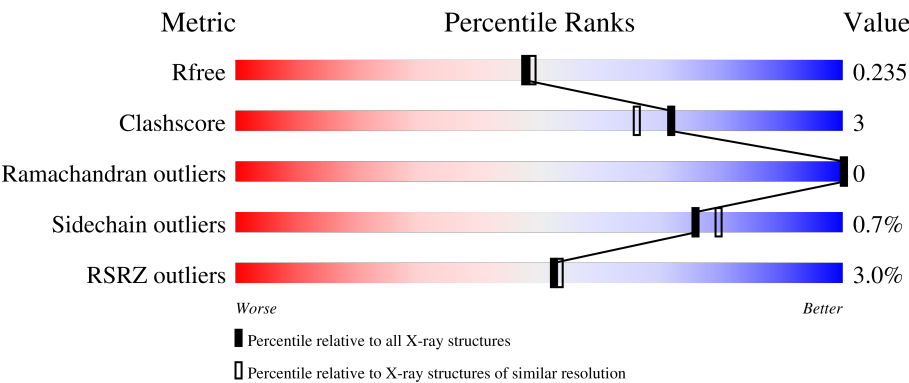
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	270	2% 87% 5% 7%
1	B	270	% 86% 7% 7%
1	C	270	% 85% 7% 7%
1	D	270	% 85% 8% 7%
1	E	270	% 87% 6% 7%

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Mol	Chain	Length	Quality of chain
1	F	270	% 86% 7% 7%
1	G	270	% 83% 9% 8%
1	H	270	13% 75% 16% 9%

2 Entry composition

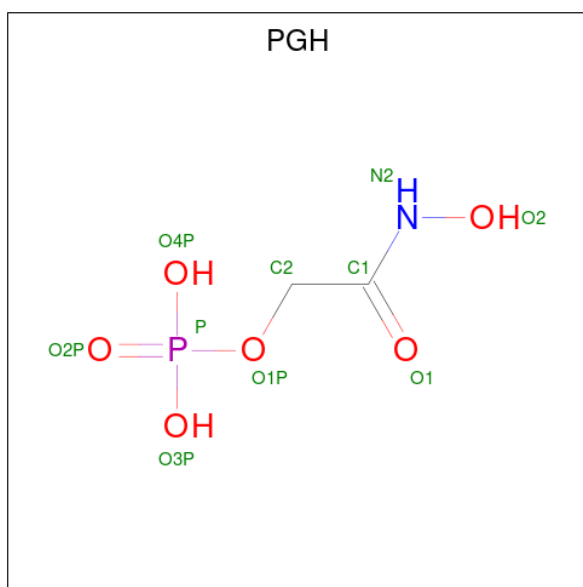
There are 10 unique types of molecules in this entry. The entry contains 16891 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Triosephosphate isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	3	0
			1950	1234	333	376	7			
1	B	251	Total	C	N	O	S	0	3	0
			1948	1232	332	377	7			
1	C	250	Total	C	N	O	S	0	4	0
			1955	1233	332	383	7			
1	D	251	Total	C	N	O	S	0	5	0
			1976	1245	337	387	7			
1	E	251	Total	C	N	O	S	0	2	0
			1948	1229	332	380	7			
1	F	251	Total	C	N	O	S	0	1	0
			1942	1226	332	377	7			
1	G	249	Total	C	N	O	S	0	0	0
			1914	1211	327	370	6			
1	H	246	Total	C	N	O	S	0	1	0
			1871	1185	323	357	6			

- Molecule 2 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: $\text{C}_2\text{H}_6\text{NO}_6\text{P}$) (labeled as "Ligand of Interest" by depositor).



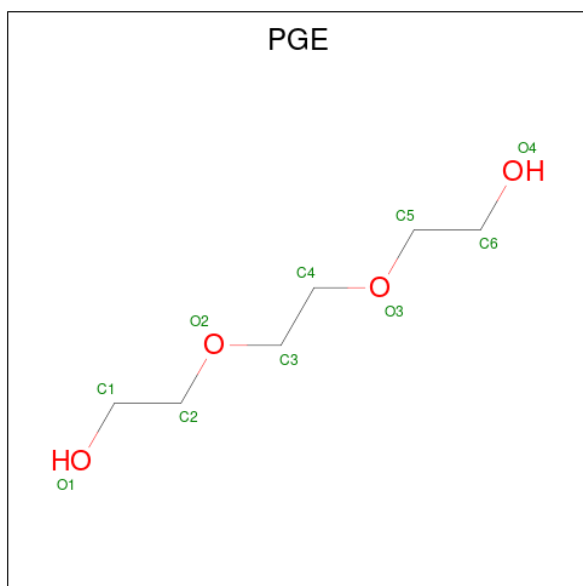
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

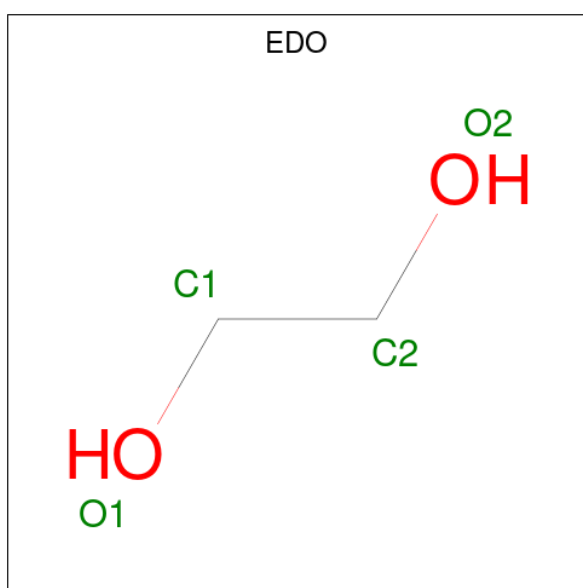


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

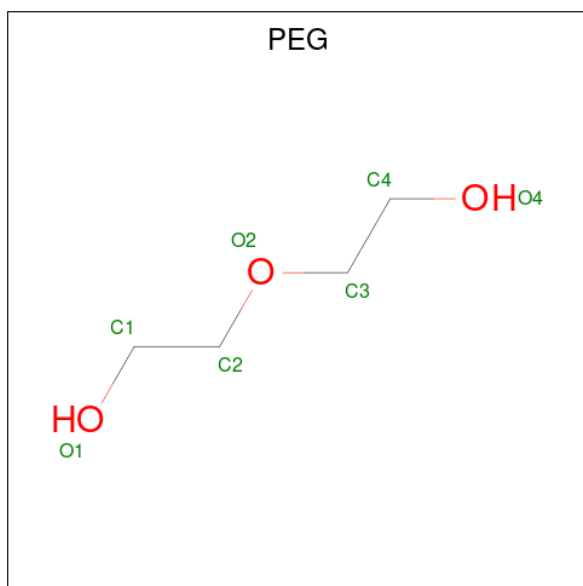
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			7	4	3		
8	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	F	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	218	Total	O	0	0
			218	218		
10	B	196	Total	O	0	0
			196	196		
10	C	182	Total	O	0	0
			182	182		

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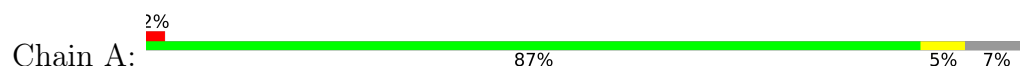
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	175	Total 175	O 175	0	0
10	E	173	Total 173	O 173	0	0
10	F	123	Total 123	O 123	0	0
10	G	135	Total 135	O 135	0	0
10	H	67	Total 67	O 67	0	0

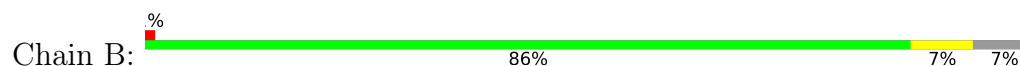
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

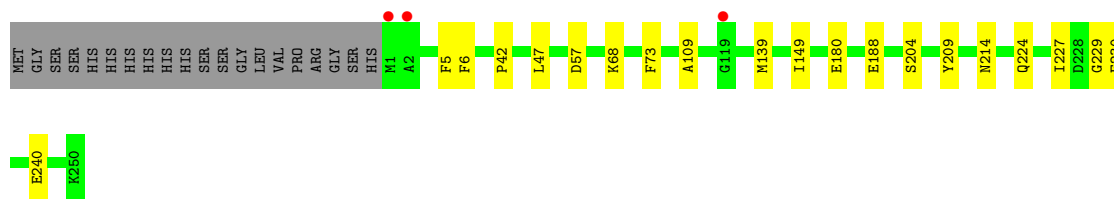
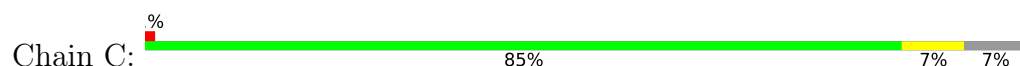
- Molecule 1: Triosephosphate isomerase



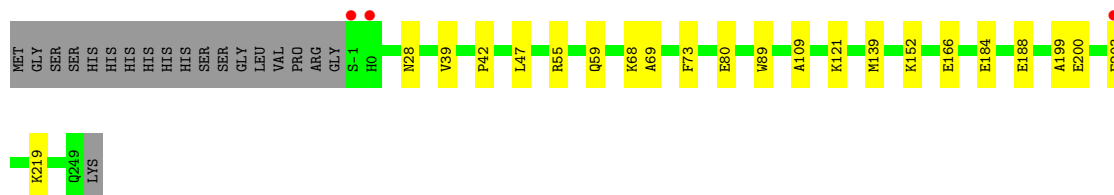
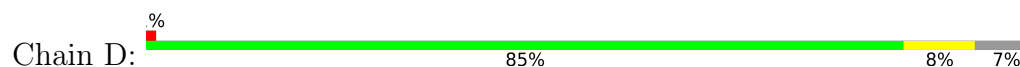
- Molecule 1: Triosephosphate isomerase



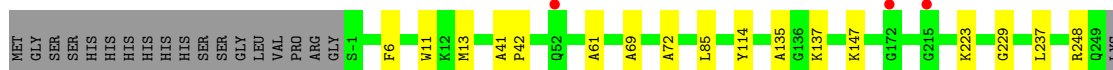
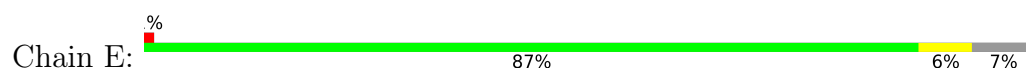
- Molecule 1: Triosephosphate isomerase



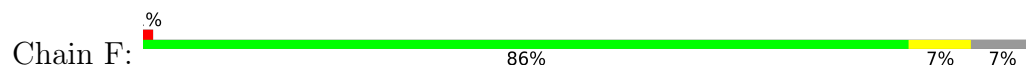
- Molecule 1: Triosephosphate isomerase



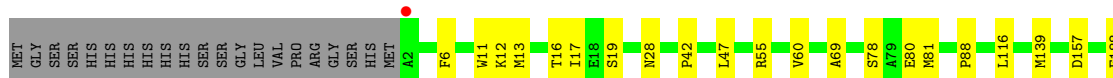
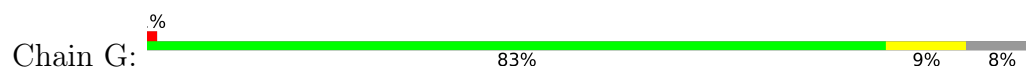
- Molecule 1: Triosephosphate isomerase



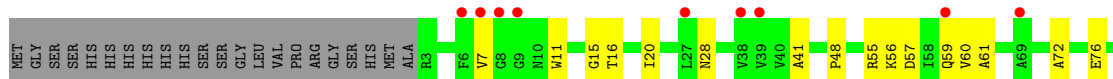
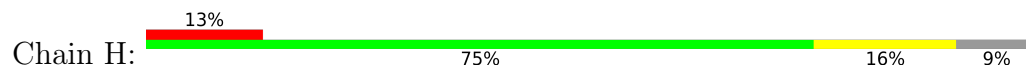
- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



- Molecule 1: Triosephosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.64Å 83.22Å 127.86Å 90.00° 103.49° 90.00°	Depositor
Resolution (Å)	41.45 – 2.06 41.45 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.5 (41.45-2.06) 99.5 (41.45-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.07Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.195 , 0.235 0.195 , 0.235	Depositor DCC
R_{free} test set	7110 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16891	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT, NA, PEG, ACY, PGE, PGH, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/1985	0.64	1/2685 (0.0%)
1	B	0.40	0/1983	0.59	0/2684
1	C	0.37	0/1986	0.53	0/2687
1	D	0.35	0/2008	0.52	0/2717
1	E	0.35	0/1980	0.52	0/2679
1	F	0.33	0/1974	0.50	0/2671
1	G	0.40	0/1945	0.56	0/2632
1	H	0.54	0/1902	0.72	3/2578 (0.1%)
All	All	0.41	0/15763	0.58	4/21333 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLY	N-CA-C	5.90	123.01	114.10
1	H	233	GLY	O-C-N	5.50	124.93	121.85
1	H	229	GLY	N-CA-C	5.35	117.14	110.29
1	H	15	GLY	N-CA-C	5.10	125.27	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1950	0	1967	8	0
1	B	1948	0	1955	11	0
1	C	1955	0	1953	10	0
1	D	1976	0	1973	12	0
1	E	1948	0	1951	13	0
1	F	1942	0	1949	13	0
1	G	1914	0	1927	15	0
1	H	1871	0	1861	26	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	1	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
3	B	4	0	3	0	0
4	C	10	0	14	1	0
5	C	4	0	3	0	0
6	D	1	0	0	0	0
7	D	4	0	6	0	0
8	E	7	0	10	0	0
8	G	7	0	10	0	0
9	F	1	0	0	0	0
10	A	218	0	0	0	0
10	B	196	0	0	2	0
10	C	182	0	0	1	0
10	D	175	0	0	0	0
10	E	173	0	0	4	0
10	F	123	0	0	1	0
10	G	135	0	0	0	0
10	H	67	0	0	0	0
All	All	16891	0	15614	103	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:153:ILE:HD11	1:H:158:TRP:CE2	2.16	0.80
1:H:139:MET:HE1	1:H:185:VAL:HG13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:GLU:HA	1:H:223:LYS:HD2	1.74	0.69
1:H:28:ASN:HA	1:H:55:ARG:HD2	1.73	0.68
1:F:48:PRO:O	1:F:52[A]:GLN:HG2	1.99	0.61
1:E:147:LYS:HD3	10:E:428:HOH:O	2.01	0.60
1:G:42:PRO:HG2	1:G:47:LEU:HD23	1.86	0.58
1:F:121:LYS:HG2	1:F:160:LYS:HE2	1.84	0.58
1:C:42:PRO:HG2	1:C:47:LEU:HD23	1.86	0.57
1:A:1:MET:HE3	10:C:534:HOH:O	2.04	0.57
1:D:109:ALA:HB1	1:D:152:LYS:HD2	1.85	0.57
1:G:16:THR:H	1:G:19:SER:HB2	1.69	0.57
1:H:55:ARG:HB2	1:H:57:ASP:OD1	2.05	0.56
1:E:6:PHE:O	1:E:229:GLY:HA3	2.07	0.55
1:F:160:LYS:HD3	10:F:431:HOH:O	2.07	0.55
1:G:17:ILE:HD11	1:H:85:LEU:HD12	1.89	0.55
1:H:219:LYS:HG3	1:H:247:ALA:O	2.07	0.55
1:E:11:TRP:CZ3	1:E:42:PRO:HB3	2.42	0.55
1:E:72:ALA:HA	1:F:12:LYS:HD3	1.89	0.55
1:H:153:ILE:HD11	1:H:158:TRP:CD2	2.42	0.54
1:D:184:GLU:O	1:D:188:GLU:HG2	2.07	0.54
1:E:85:LEU:HD22	1:F:45:ILE:HD11	1.89	0.54
1:H:123:ILE:HA	1:H:162:VAL:HG13	1.89	0.54
1:G:11:TRP:CZ3	1:G:42:PRO:HB3	2.42	0.53
1:A:28:ASN:HA	1:A:55:ARG:HD2	1.92	0.52
1:H:116:LEU:HD13	1:H:157:ASP:HB3	1.93	0.51
1:H:59[B]:GLN:HG2	1:H:88:PRO:HG2	1.93	0.51
1:F:180:GLU:H	1:F:180:GLU:CD	2.19	0.51
1:G:28:ASN:HA	1:G:55:ARG:HD2	1.92	0.51
1:D:199:ALA:O	1:D:203:GLU:HG2	2.12	0.50
1:G:11:TRP:CE3	1:G:42:PRO:HB3	2.46	0.50
1:D:139:MET:HE3	1:D:139:MET:HA	1.92	0.50
1:H:57:ASP:OD1	1:H:57:ASP:N	2.45	0.50
1:A:246:ASN:HB3	1:A:249:GLN:HG2	1.94	0.50
1:G:139:MET:HE2	1:G:188:GLU:HB3	1.92	0.50
1:B:42:PRO:HG2	1:B:47:LEU:HD23	1.94	0.49
1:B:56:LYS:HE2	10:B:483:HOH:O	2.12	0.49
1:H:176:VAL:HG22	1:H:177:ALA:O	2.13	0.49
1:H:11:TRP:CZ3	1:H:20:ILE:HD12	2.47	0.49
1:F:155:GLU:H	1:F:155:GLU:CD	2.21	0.48
1:H:7:VAL:HG21	1:H:245:ILE:HA	1.94	0.48
1:B:17:ILE:HG22	1:B:21:LYS:HD2	1.93	0.48
1:G:13:MET:HG3	1:H:76:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:MET:HE2	1:F:188:GLU:HB3	1.95	0.48
1:E:135:ALA:CB	1:E:137:LYS:HE3	2.44	0.48
1:C:139:MET:HE2	1:C:188:GLU:HB3	1.95	0.47
1:E:237:LEU:HD12	10:E:525:HOH:O	2.14	0.47
1:D:89:TRP:CE2	1:D:121:LYS:HE3	2.49	0.47
1:G:78:SER:OG	1:G:81:MET:HG3	2.15	0.47
1:H:41:ALA:HB2	1:H:61:ALA:HB3	1.95	0.47
1:E:69:ALA:HB2	1:E:114:TYR:OH	2.14	0.47
1:H:167:PRO:HB2	1:H:169:TRP:CE2	2.50	0.47
1:E:135:ALA:HB1	1:E:137:LYS:HE3	1.97	0.46
1:A:6:PHE:O	1:A:229:GLY:HA3	2.15	0.46
1:G:219:LYS:HE2	1:G:250:LYS:HD2	1.97	0.46
1:G:69:ALA:HA	1:G:80:GLU:OE1	2.15	0.46
1:C:214:ASN:HB2	1:C:240:GLU:OE2	2.15	0.46
1:E:223:LYS:NZ	10:E:408:HOH:O	2.49	0.46
1:G:116:LEU:HD13	1:G:157:ASP:HB3	1.97	0.46
4:C:302:PGE:H52	4:C:302:PGE:H32	1.64	0.45
1:H:191:LYS:HD3	1:H:195:GLU:OE2	2.15	0.45
1:C:68:LYS:HD2	1:C:73:PHE:CZ	2.51	0.45
1:A:83[A]:LYS:HA	1:A:83[A]:LYS:HD2	1.59	0.45
1:C:109:ALA:HA	1:C:149:ILE:HG13	1.98	0.45
1:B:6:PHE:O	1:B:229:GLY:HA3	2.16	0.45
1:E:41:ALA:HA	1:E:61:ALA:O	2.17	0.45
1:G:12:LYS:HD3	1:H:72:ALA:HA	1.98	0.45
1:B:139[A]:MET:HE2	1:B:188:GLU:CB	2.48	0.44
1:B:106:GLU:O	1:B:110:GLU:HG3	2.18	0.44
1:B:139[A]:MET:HE2	1:B:188:GLU:HB2	1.98	0.44
1:H:107:PHE:CE2	1:H:111:LYS:HE3	2.53	0.44
1:D:69:ALA:HA	1:D:80:GLU:OE1	2.18	0.44
1:B:107:PHE:CE2	1:B:111:LYS:HE3	2.53	0.43
1:D:28:ASN:HA	1:D:55:ARG:HD2	2.01	0.43
1:F:28:ASN:HA	1:F:55:ARG:HD2	1.99	0.43
1:G:60:VAL:O	1:G:88:PRO:HD2	2.18	0.43
1:B:11:TRP:CZ3	1:B:42:PRO:HB3	2.54	0.43
1:C:209:TYR:O	1:C:230:PHE:HA	2.19	0.43
1:E:13:MET:HG3	1:F:76:GLU:O	2.18	0.43
1:C:224:GLN:HB2	1:C:227:ILE:HD12	2.00	0.42
1:F:6:PHE:O	1:F:229:GLY:HA3	2.18	0.42
1:D:68:LYS:HD2	1:D:73:PHE:CZ	2.54	0.42
1:F:199:ALA:O	1:F:203:GLU:HG3	2.19	0.42
1:D:166[A]:GLU:OE2	2:D:302:PGH:N2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:VAL:HA	1:D:59[A]:GLN:O	2.19	0.42
1:D:200:GLU:CD	1:D:200:GLU:H	2.27	0.42
1:A:126:ILE:HD13	1:A:146[A]:LEU:HG	2.00	0.42
1:C:6:PHE:O	1:C:229:GLY:HA3	2.19	0.42
1:H:60:VAL:O	1:H:88:PRO:HD2	2.20	0.42
1:B:224:GLN:NE2	10:B:416:HOH:O	2.52	0.42
1:G:6:PHE:O	1:G:229:GLY:HA3	2.19	0.42
1:C:5:PHE:CE1	1:C:229:GLY:HA2	2.55	0.41
1:D:42:PRO:HG2	1:D:47:LEU:HD23	2.01	0.41
1:A:11:TRP:CZ3	1:A:42:PRO:HB3	2.55	0.41
1:H:48:PRO:HG3	1:H:85:LEU:HD21	2.02	0.41
1:A:146[A]:LEU:HD23	1:A:146[A]:LEU:HA	1.94	0.41
1:C:57:ASP:OD1	1:C:57:ASP:N	2.54	0.41
1:E:248:ARG:HD3	10:E:406:HOH:O	2.20	0.41
1:H:155:GLU:HA	1:H:158:TRP:HD1	1.86	0.41
1:B:69:ALA:HA	1:B:80:GLU:OE1	2.21	0.40
1:H:16:THR:O	1:H:20:ILE:HG12	2.21	0.40
1:F:146:LEU:HD23	1:F:146:LEU:HA	1.94	0.40
1:H:123:ILE:HG12	1:H:162:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/270 (93%)	241 (96%)	10 (4%)	0	100	100
1	B	252/270 (93%)	243 (96%)	9 (4%)	0	100	100
1	C	252/270 (93%)	245 (97%)	7 (3%)	0	100	100
1	D	254/270 (94%)	246 (97%)	8 (3%)	0	100	100
1	E	251/270 (93%)	245 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	250/270 (93%)	242 (97%)	8 (3%)	0	100	100
1	G	247/270 (92%)	240 (97%)	7 (3%)	0	100	100
1	H	245/270 (91%)	234 (96%)	11 (4%)	0	100	100
All	All	2002/2160 (93%)	1936 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/222 (94%)	206 (99%)	2 (1%)	68	71
1	B	207/222 (93%)	206 (100%)	1 (0%)	81	85
1	C	208/222 (94%)	205 (99%)	3 (1%)	59	60
1	D	211/222 (95%)	210 (100%)	1 (0%)	81	85
1	E	208/222 (94%)	208 (100%)	0	100	100
1	F	207/222 (93%)	206 (100%)	1 (0%)	81	85
1	G	203/222 (91%)	202 (100%)	1 (0%)	81	85
1	H	194/222 (87%)	190 (98%)	4 (2%)	47	45
All	All	1646/1776 (93%)	1633 (99%)	13 (1%)	76	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	1	MET
1	B	166	GLU
1	C	180[A]	GLU
1	C	180[B]	GLU
1	C	204	SER
1	D	219	LYS
1	F	83	LYS

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Mol	Chain	Res	Type
1	G	250	LYS
1	H	56	LYS
1	H	85	LEU
1	H	156	SER
1	H	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	B	186	HIS
1	B	249	GLN
1	C	196	ASN
1	C	224	GLN
1	D	224	GLN
1	D	249	GLN
1	E	118	ASN
1	F	59	GLN
1	H	99	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	B	302	-	3,3,3	1.66	0	3,3,3	1.71	1 (33%)
2	PGH	C	301	-	9,9,9	0.76	0	10,12,12	0.88	0
7	EDO	D	303	-	3,3,3	0.48	0	2,2,2	0.37	0
2	PGH	A	301	-	9,9,9	0.81	0	10,12,12	0.94	0
2	PGH	D	302	-	9,9,9	0.79	0	10,12,12	0.88	0
4	PGE	C	302	-	9,9,9	0.28	0	8,8,8	0.40	0
2	PGH	E	301	-	9,9,9	0.77	0	10,12,12	0.98	0
5	ACT	C	303	-	3,3,3	1.22	0	3,3,3	1.46	1 (33%)
2	PGH	B	301	-	9,9,9	0.81	0	10,12,12	0.95	0
2	PGH	G	301	-	9,9,9	0.76	0	10,12,12	0.90	0
2	PGH	H	301	-	9,9,9	0.75	0	10,12,12	0.93	1 (10%)
8	PEG	G	302	-	6,6,6	0.11	0	5,5,5	0.12	0
2	PGH	F	302	-	9,9,9	0.74	0	10,12,12	0.92	0
8	PEG	E	302	-	6,6,6	0.16	0	5,5,5	0.08	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGH	C	301	-	-	2/8/8/8	-
7	EDO	D	303	-	-	0/1/1/1	-
2	PGH	A	301	-	-	2/8/8/8	-
2	PGH	D	302	-	-	4/8/8/8	-
4	PGE	C	302	-	-	4/7/7/7	-
2	PGH	E	301	-	-	2/8/8/8	-
2	PGH	B	301	-	-	2/8/8/8	-
2	PGH	G	301	-	-	1/8/8/8	-
2	PGH	H	301	-	-	3/8/8/8	-
8	PEG	G	302	-	-	3/4/4/4	-
2	PGH	F	302	-	-	2/8/8/8	-
8	PEG	E	302	-	-	1/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	ACY	O-C-CH3	-2.33	112.95	122.53
2	H	301	PGH	O4P-P-O3P	2.01	115.34	107.80
5	C	303	ACT	OXT-C-O	2.00	129.45	122.03

There are no chirality outliers.

All (26) torsion outliers are listed below:

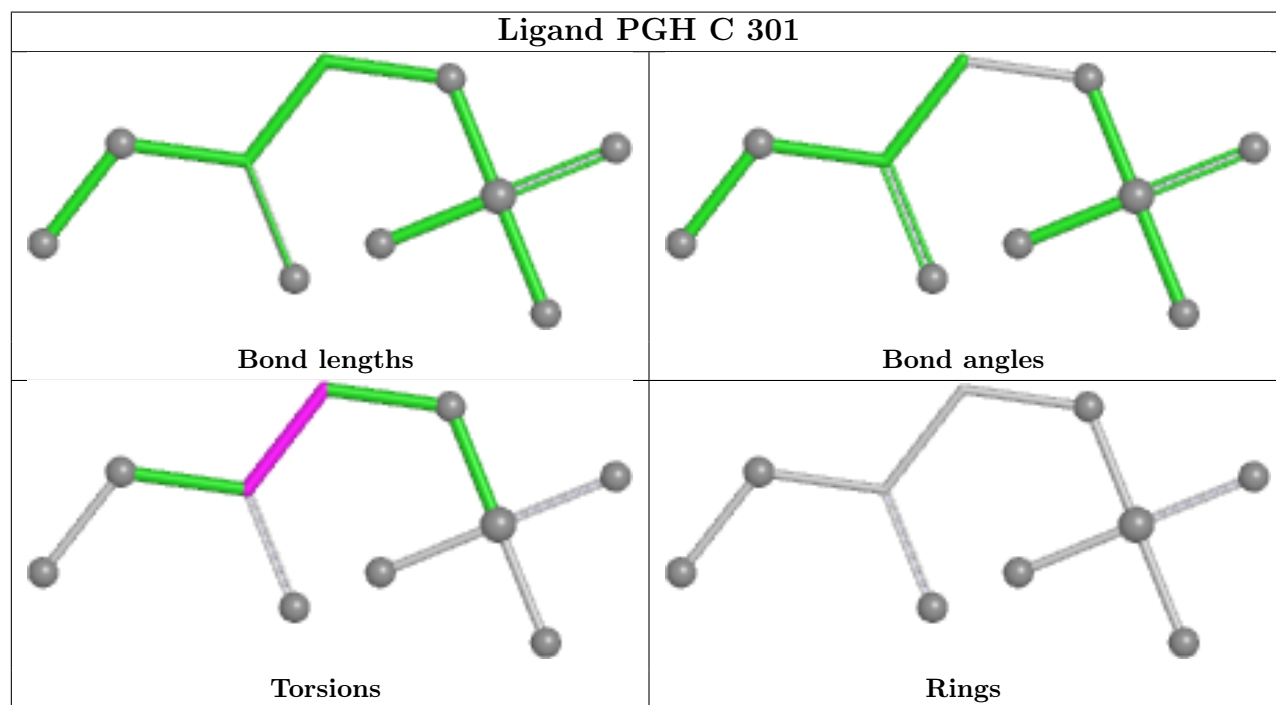
Mol	Chain	Res	Type	Atoms
2	A	301	PGH	N2-C1-C2-O1P
2	C	301	PGH	N2-C1-C2-O1P
2	D	302	PGH	C2-C1-N2-O2
2	D	302	PGH	O1-C1-N2-O2
2	E	301	PGH	N2-C1-C2-O1P
2	H	301	PGH	C2-C1-N2-O2
2	H	301	PGH	O1-C1-N2-O2
4	C	302	PGE	C3-C4-O3-C5
4	C	302	PGE	O2-C3-C4-O3
8	G	302	PEG	O2-C3-C4-O4
8	G	302	PEG	O1-C1-C2-O2
2	D	302	PGH	C2-O1P-P-O2P
2	A	301	PGH	O1-C1-C2-O1P
2	C	301	PGH	O1-C1-C2-O1P
2	F	302	PGH	O1-C1-C2-O1P
2	B	301	PGH	O1-C1-C2-O1P
2	D	302	PGH	O1-C1-C2-O1P
2	E	301	PGH	O1-C1-C2-O1P
2	G	301	PGH	O1-C1-C2-O1P
2	F	302	PGH	N2-C1-C2-O1P
4	C	302	PGE	O1-C1-C2-O2
4	C	302	PGE	C1-C2-O2-C3
2	B	301	PGH	C2-O1P-P-O2P
8	G	302	PEG	C1-C2-O2-C3
2	H	301	PGH	O1-C1-C2-O1P
8	E	302	PEG	O2-C3-C4-O4

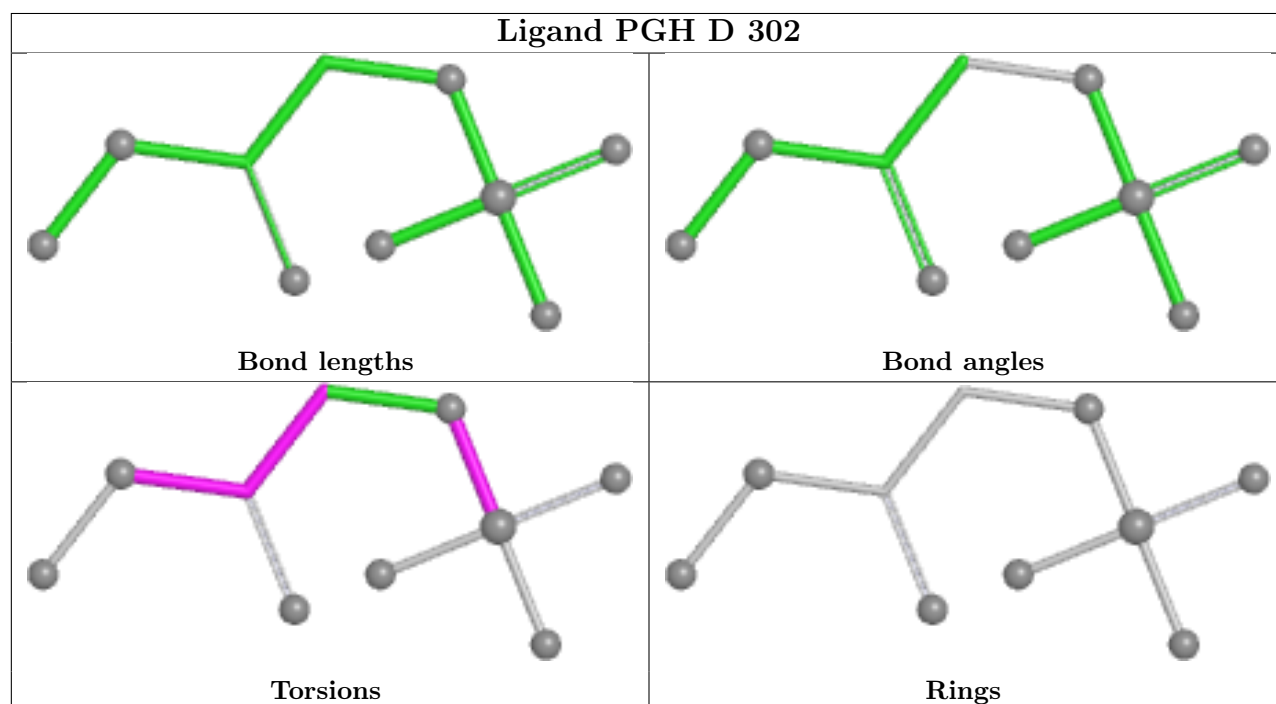
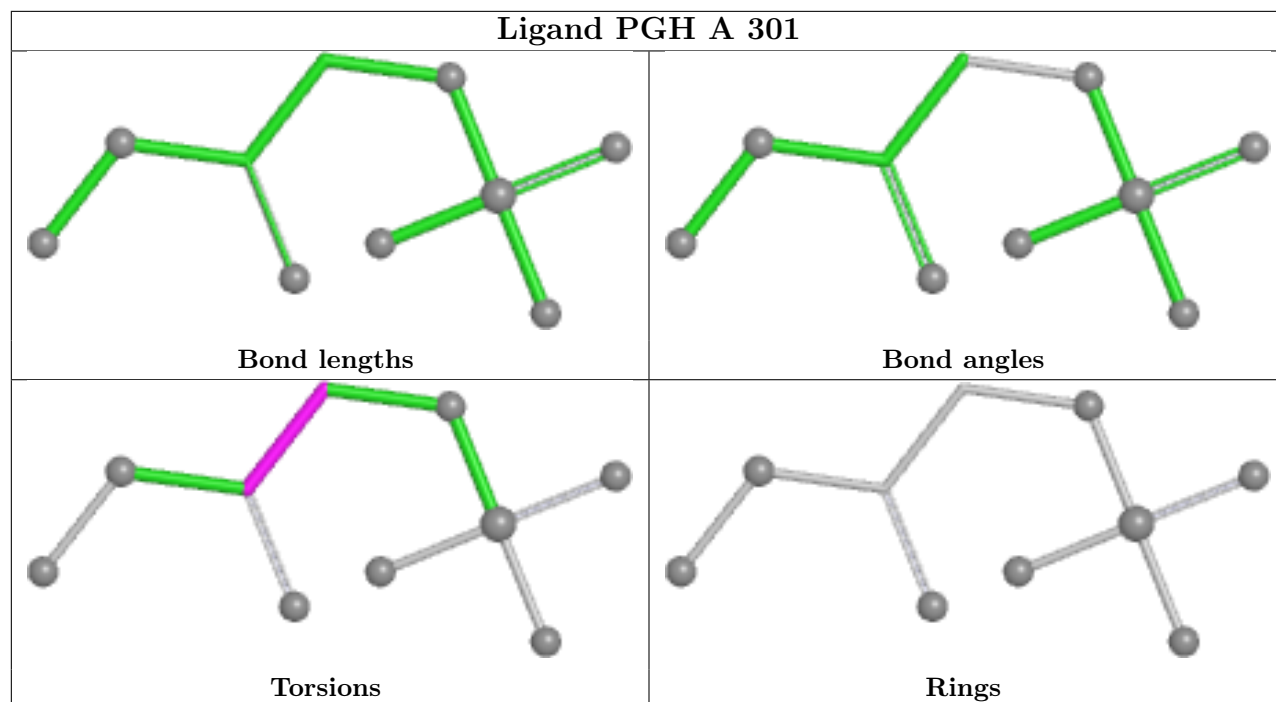
There are no ring outliers.

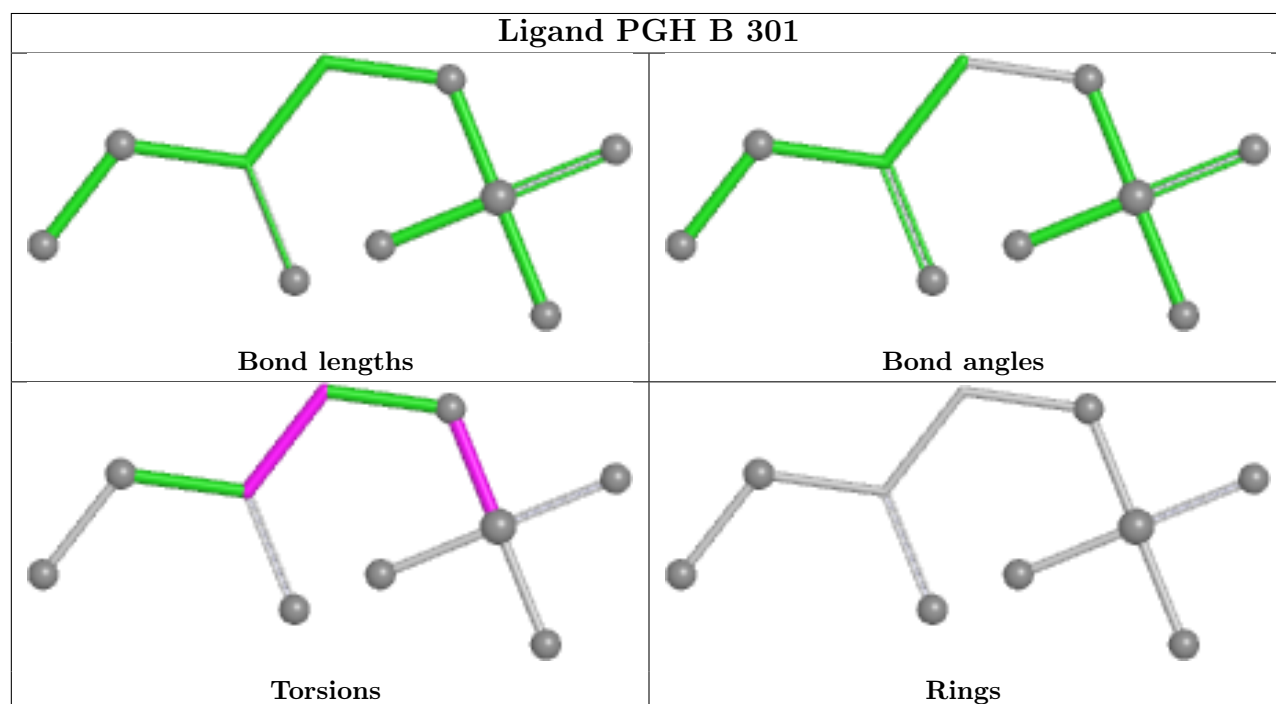
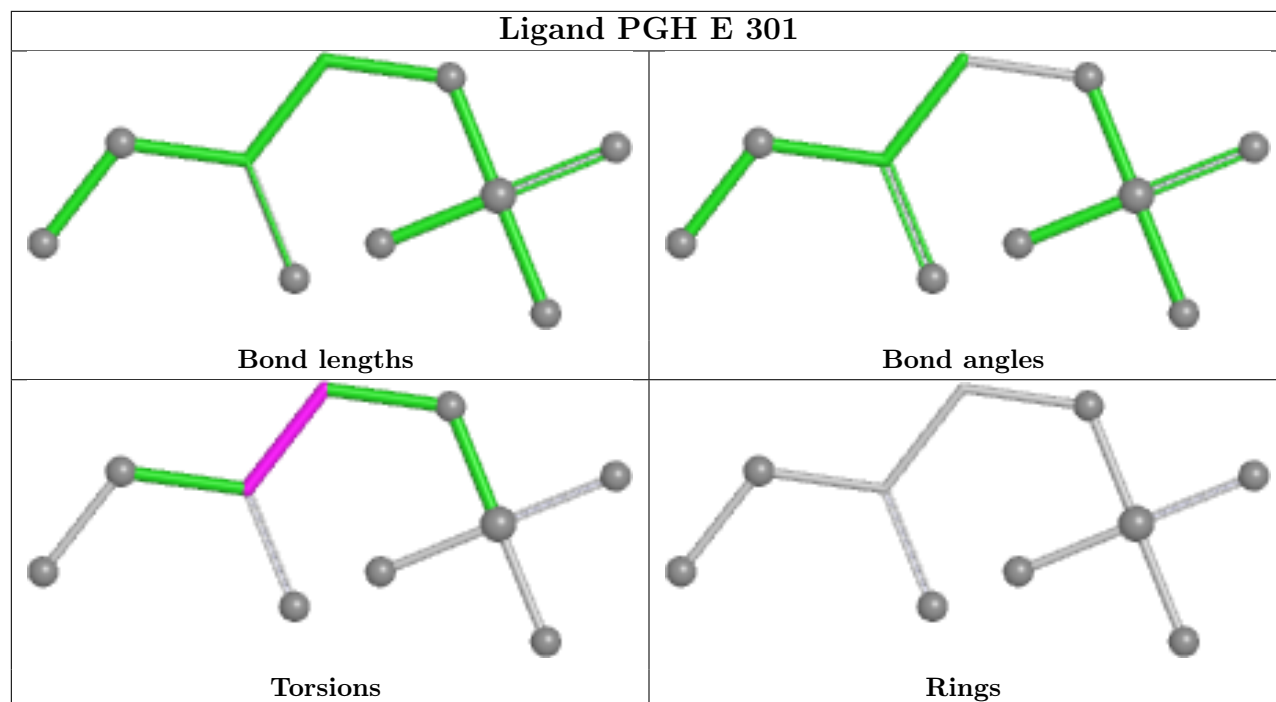
2 monomers are involved in 2 short contacts:

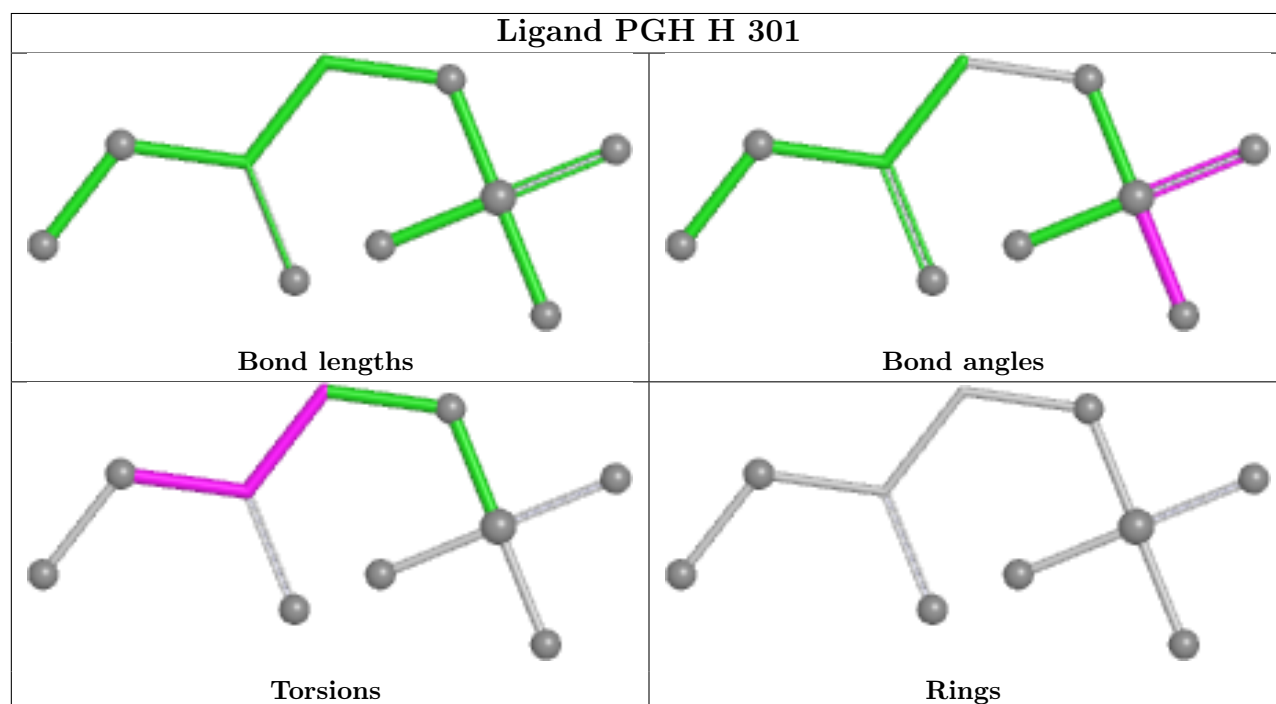
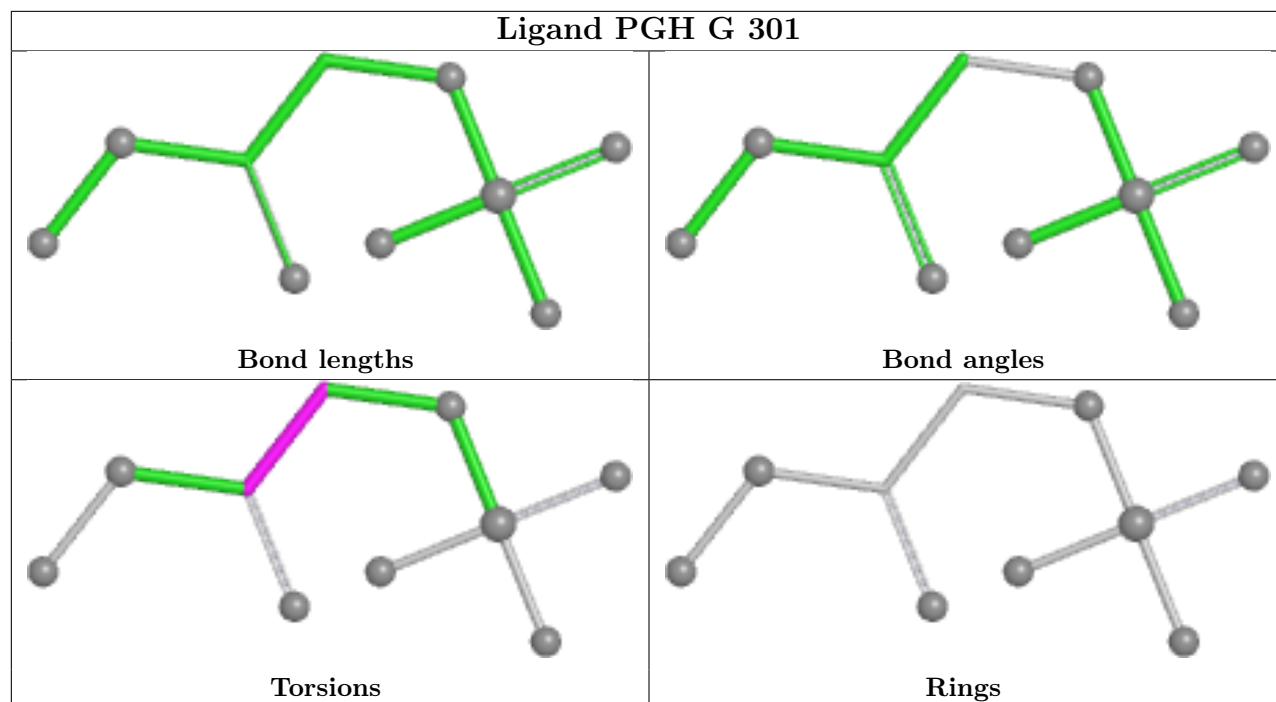
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	302	PGH	1	0
4	C	302	PGE	1	0

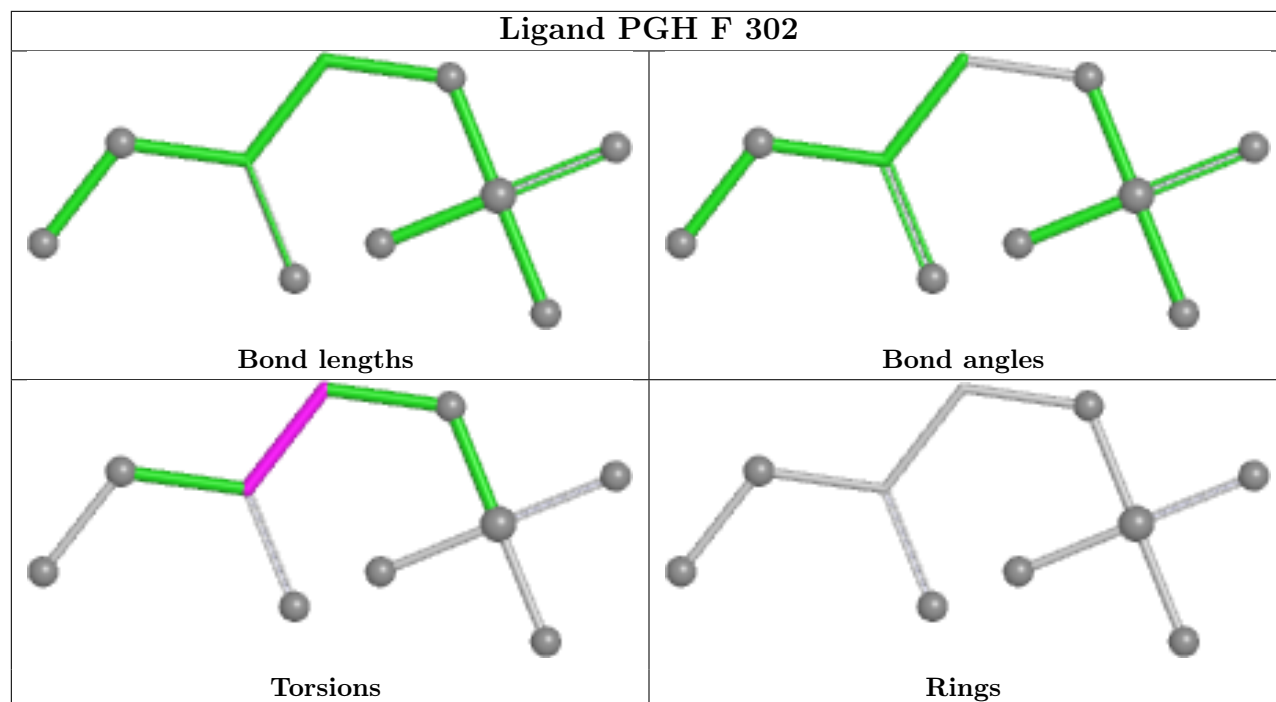
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/270 (92%)	0.07	5 (2%) 65 67	9, 23, 39, 60	3 (1%)
1	B	251/270 (92%)	0.11	4 (1%) 70 73	11, 25, 43, 69	3 (1%)
1	C	250/270 (92%)	-0.00	3 (1%) 76 78	13, 25, 39, 73	4 (1%)
1	D	251/270 (92%)	0.05	3 (1%) 76 78	12, 26, 41, 63	5 (1%)
1	E	251/270 (92%)	0.28	3 (1%) 76 78	14, 30, 44, 57	2 (0%)
1	F	251/270 (92%)	0.36	4 (1%) 70 73	19, 33, 46, 68	1 (0%)
1	G	249/270 (92%)	0.24	2 (0%) 82 84	21, 31, 43, 57	0
1	H	246/270 (91%)	1.15	35 (14%) 6 6	23, 45, 61, 72	1 (0%)
All	All	1999/2160 (92%)	0.28	59 (2%) 52 53	9, 29, 50, 73	19 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.6
1	C	1	MET	4.1
1	B	1	MET	3.9
1	A	0	HIS	3.7
1	H	69	ALA	3.6
1	H	198	SER	3.5
1	H	245	ILE	3.4
1	H	197	VAL	3.3
1	C	2	ALA	3.3
1	H	89	TRP	3.3
1	H	8	GLY	3.2
1	H	162	VAL	3.1
1	H	227	ILE	3.1
1	H	9	GLY	3.0
1	A	2	ALA	3.0
1	B	2	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	166	GLU	2.9
1	F	0	HIS	2.9
1	E	215	GLY	2.8
1	H	247	ALA	2.8
1	H	242	VAL	2.8
1	D	-1	SER	2.8
1	H	6	PHE	2.7
1	H	230	PHE	2.6
1	H	180	GLU	2.6
1	D	0	HIS	2.6
1	H	120	LEU	2.6
1	H	38	VAL	2.5
1	A	52	GLN	2.4
1	H	179	PRO	2.4
1	F	-1	SER	2.4
1	H	232	VAL	2.4
1	H	39	VAL	2.4
1	H	222	ALA	2.3
1	E	52	GLN	2.3
1	G	2	ALA	2.3
1	H	194	ALA	2.3
1	C	119	GLY	2.3
1	H	155	GLU	2.2
1	H	213	VAL	2.2
1	H	199	ALA	2.2
1	H	27	LEU	2.2
1	A	31	GLU	2.2
1	H	59[A]	GLN	2.2
1	H	192	TRP	2.2
1	H	157	ASP	2.2
1	H	87	ILE	2.1
1	F	52[A]	GLN	2.1
1	B	0	HIS	2.1
1	F	2	ALA	2.1
1	D	203	GLU	2.1
1	H	216	GLY	2.1
1	H	150	ALA	2.1
1	H	205	THR	2.1
1	H	204	SER	2.1
1	G	215	GLY	2.0
1	H	7	VAL	2.0
1	B	139[A]	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	172	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

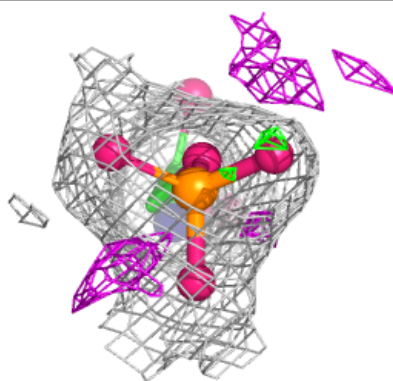
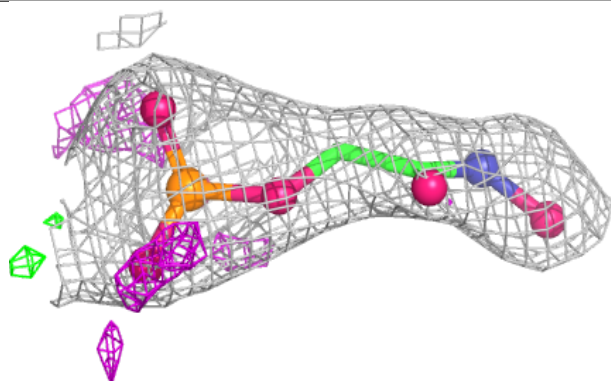
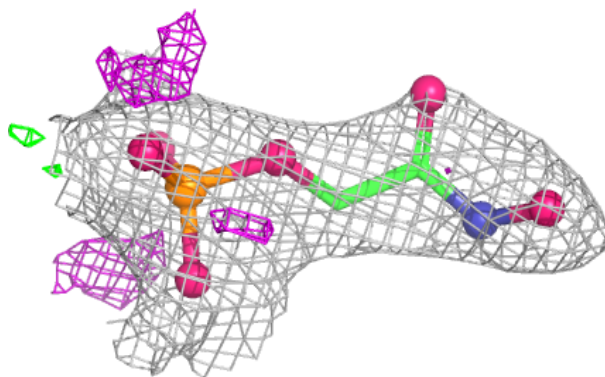
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACY	B	302	4/4	0.71	0.17	41,46,59,63	0
7	EDO	D	303	4/4	0.78	0.15	42,44,47,47	0
4	PGE	C	302	10/10	0.82	0.12	37,46,54,58	0
8	PEG	G	302	7/7	0.82	0.12	43,48,57,62	0
8	PEG	E	302	7/7	0.85	0.12	49,55,58,59	0
5	ACT	C	303	4/4	0.88	0.09	43,52,54,54	0
2	PGH	H	301	10/10	0.88	0.12	41,45,54,55	0
6	NA	D	301	1/1	0.91	0.07	21,21,21,21	0
2	PGH	F	302	10/10	0.92	0.10	31,35,41,45	0
2	PGH	E	301	10/10	0.94	0.08	26,35,39,39	0
2	PGH	G	301	10/10	0.94	0.08	27,33,39,41	0
2	PGH	D	302	10/10	0.95	0.08	24,25,35,36	0
2	PGH	A	301	10/10	0.96	0.09	21,25,33,34	0
2	PGH	B	301	10/10	0.96	0.06	24,27,34,37	0
2	PGH	C	301	10/10	0.97	0.07	22,27,33,37	0
9	CL	F	301	1/1	0.98	0.04	28,28,28,28	0

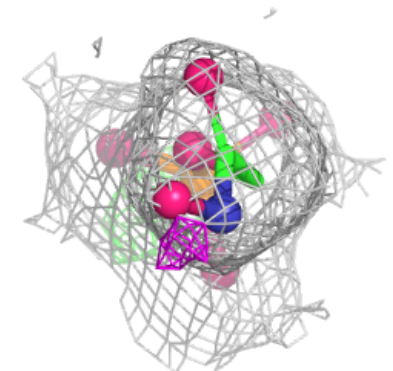
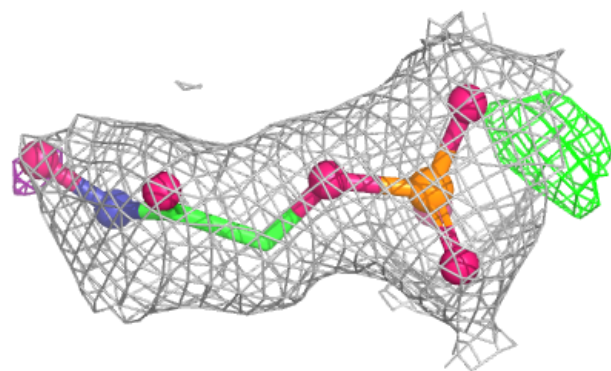
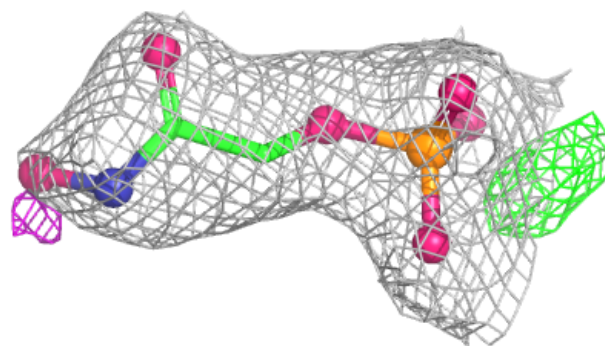
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PGH H 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

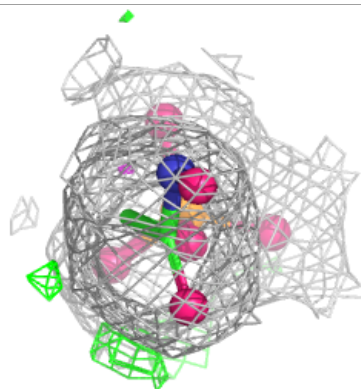
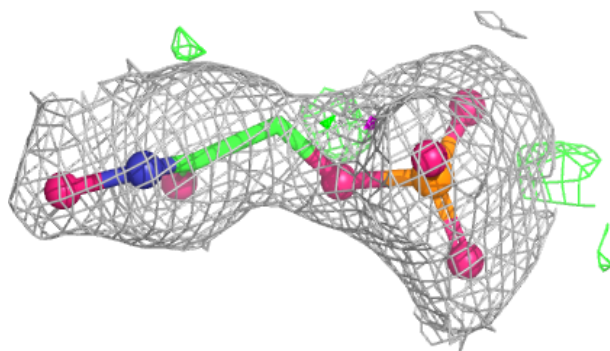
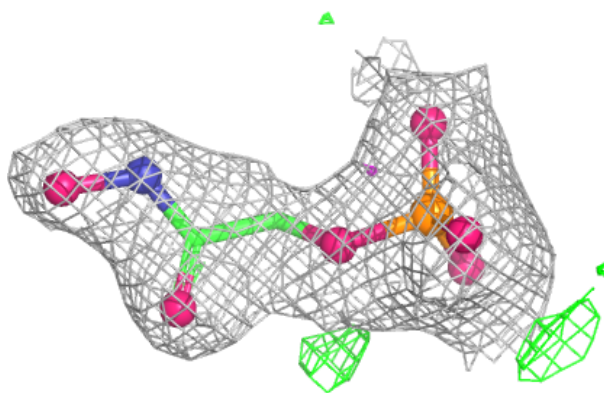
**Electron density around PGH F 302:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

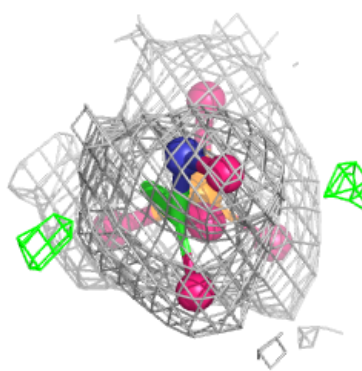
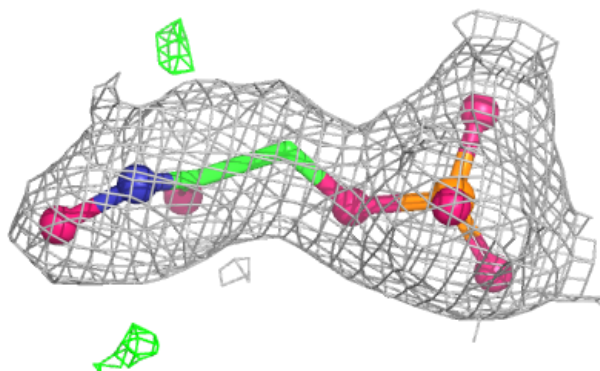
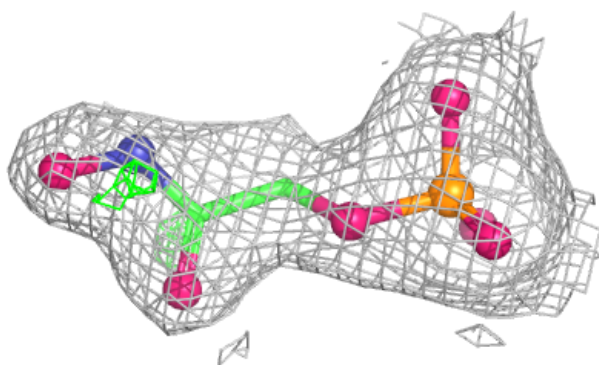


Electron density around PGH E 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

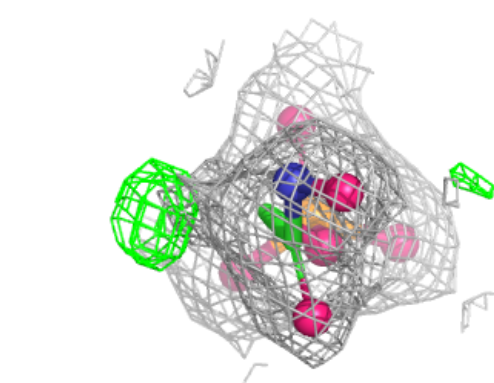
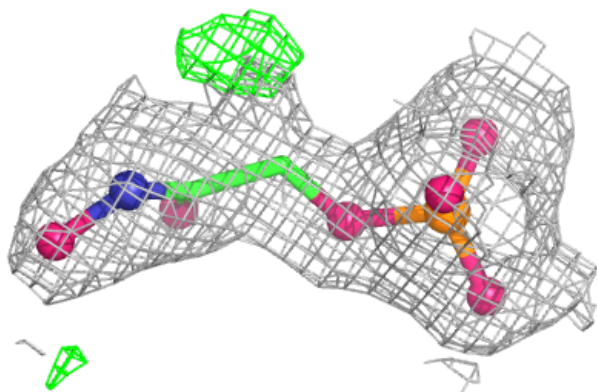
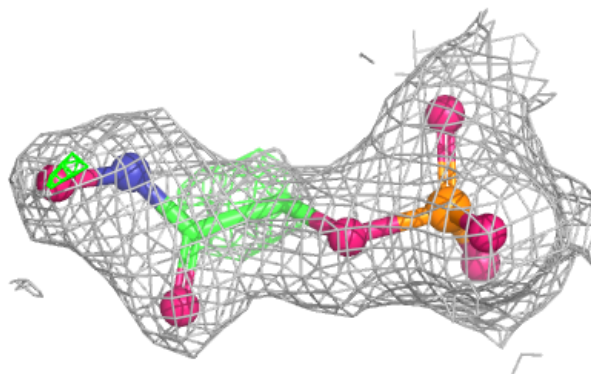
**Electron density around PGH G 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

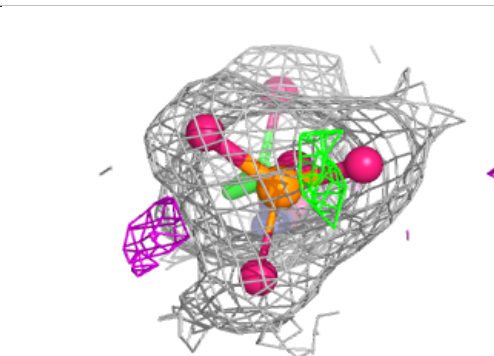
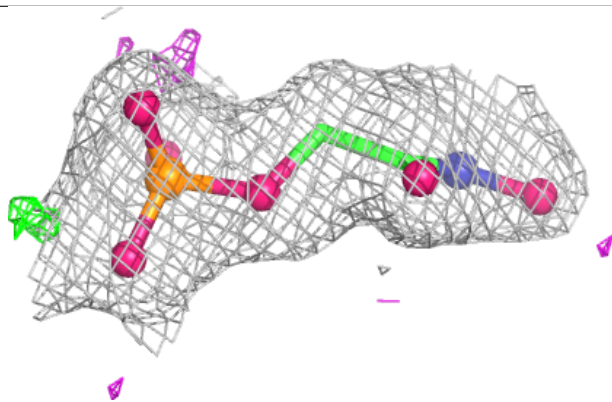
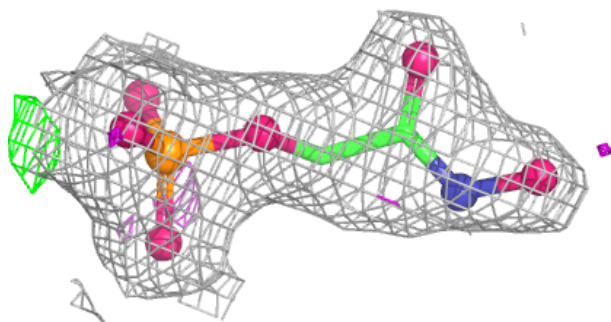


Electron density around PGH D 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

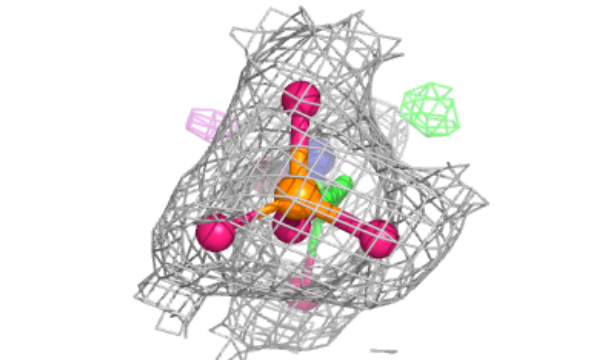
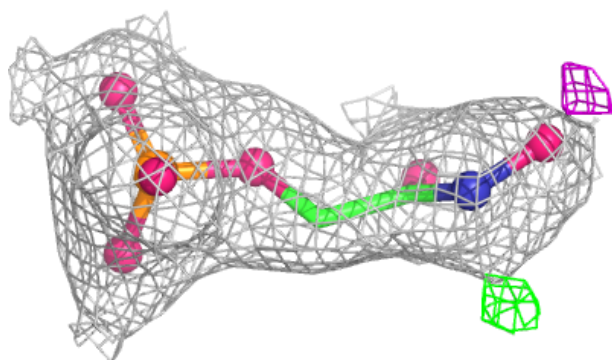
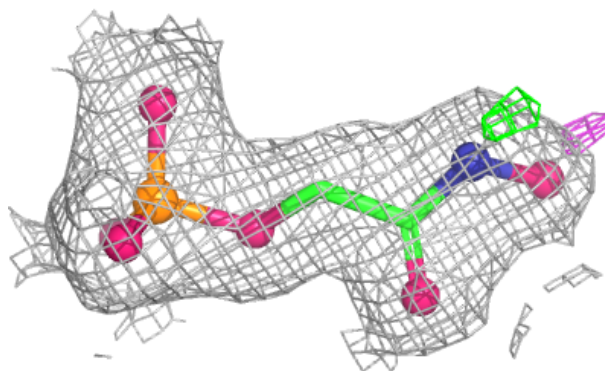
**Electron density around PGH A 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

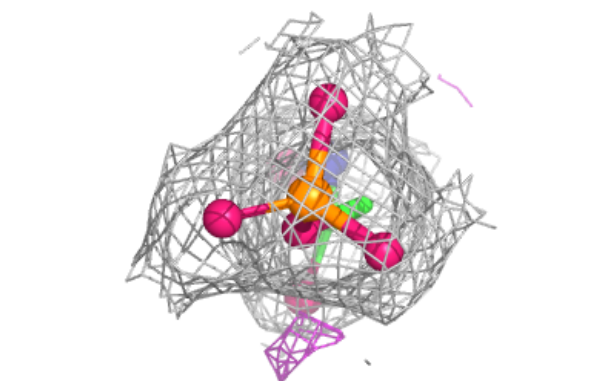
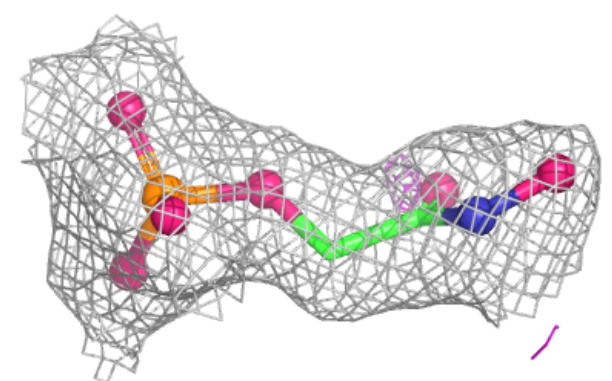
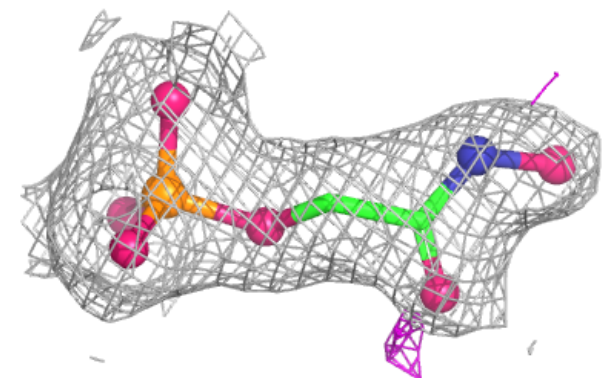


Electron density around PGH B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PGH C 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.